

Supplemental Data

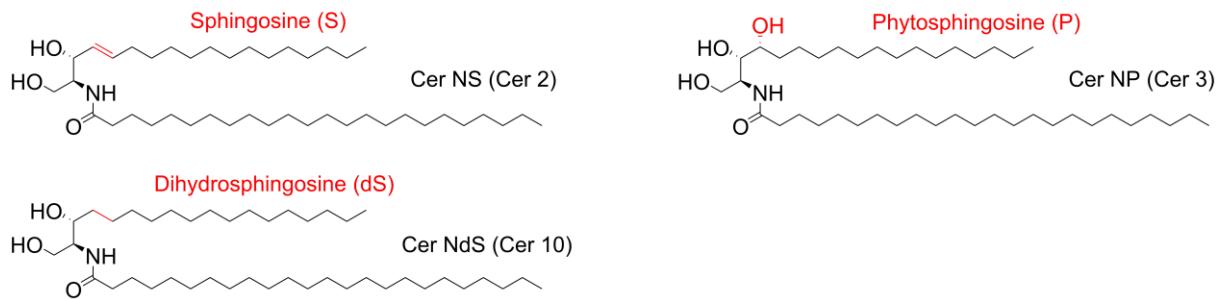
Effects of omega-*O*-acylceramide structures and concentrations in healthy and diseased skin barrier lipid membrane models

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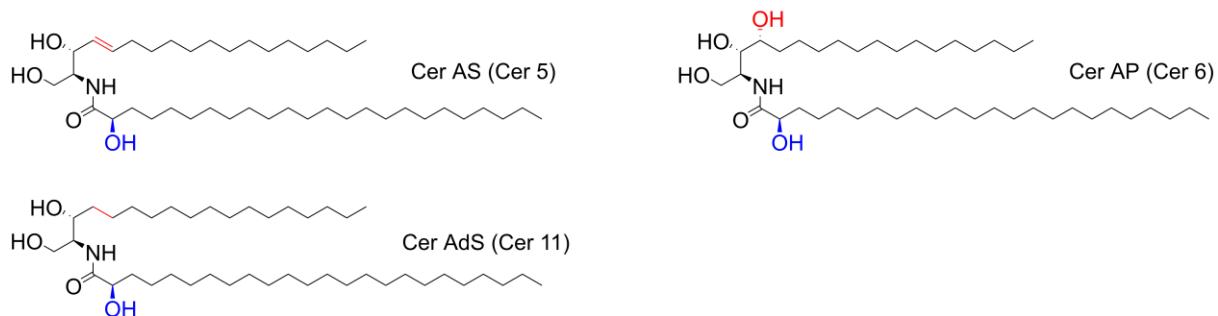
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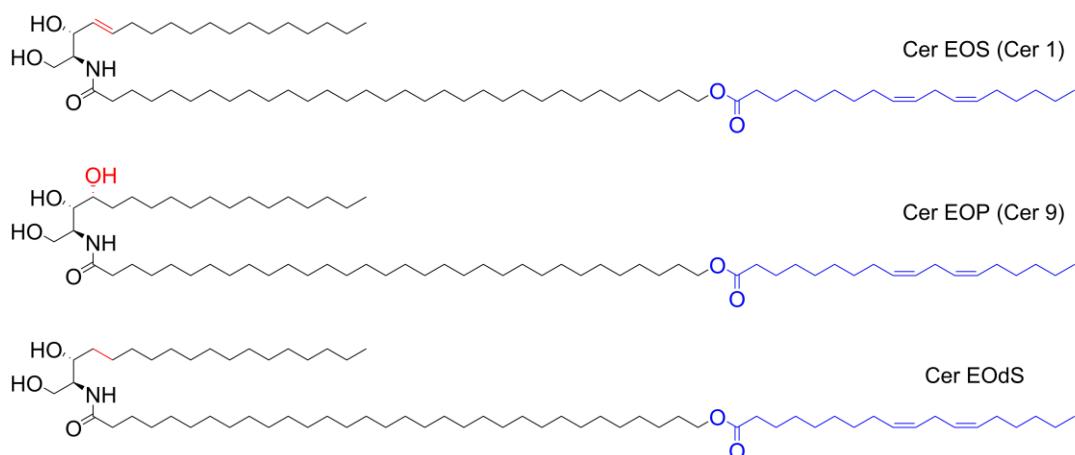
Ceramides with nonsubstituted acyl chain (N)



Ceramides with α -hydroxylated acyl chain (A)



Ceramides with ω -esterified acyl chain (EO)



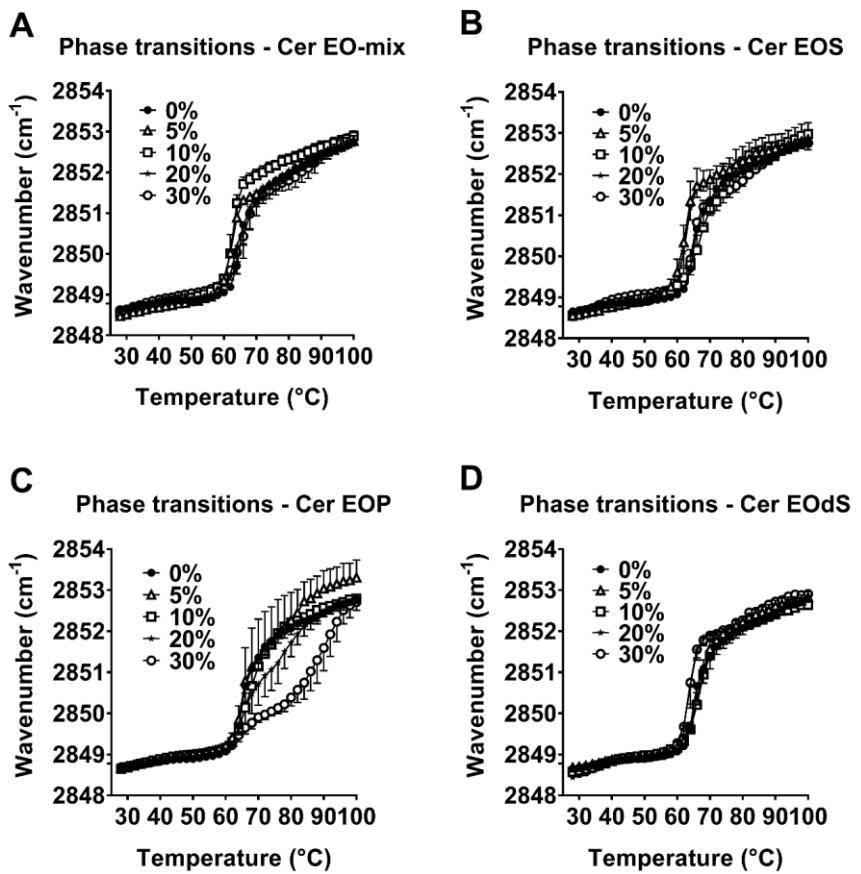
Supplemental Figure S1. Structures of Cer used for the membrane construction. SC Cer contain the following five amino alcohols called sphingoid bases: sphingosine (S), phytosphingosine (P), dihydrosphingosine (dS), 6-hydroxysphingosine (H) and dihydroxy sphinganine (T) (note: H and T-based Cer were not used in this study). The sphingoid bases are acylated on their amino group with very long nonsubstituted acid (N), very long α -hydroxylated acid (A), or ultralong ω -hydroxylated acid with linoleic acid ester-bound to the ω -hydroxyl (EO). The commonly used shorthand Cer nomenclature uses combinations of letters in parentheses.

acylCer	Molar %	Repeat distances (nm)		
		SPP	LPP	Chol
Cer EO-mix	--	5.373 ± 0.007	-	3.409 ± 0.004
	5	5.384 ± 0.017	-	3.402 ± 0.010
	10	5.377 ± 0.009	12.508 ± 0.198	3.411 ± 0.002
	20	5.378 ± 0.021	12.514 ± 0.052	3.413 ± 0.004
	30	5.387 ± 0.003	12.854 ± 0.009	3.410 ± 0.004
Cer EOS	5	5.393 ± 0.010	-	3.409 ± 0.009
	10	5.388 ± 0.016	-	3.407 ± 0.008
	20	5.380 ± 0.009	12.345 ± 0.024	3.411 ± 0.003
	30	5.359 ± 0.018	12.328 ± 0.036	3.409 ± 0.005
Cer EOP	5	5.375 ± 0.010	-	3.410 ± 0.006
	10	5.385 ± 0.007	-	3.417 ± 0.003
	20	5.350 ± 0.012	-	3.407 ± 0.008
	30	5.329 ± 0.002	12.477 ± 0.044	3.403 ± 0.010
Cer EO _d S	5	5.383 ± 0.011	-	3.414 ± 0.003
	10	5.361 ± 0.004	-	3.401 ± 0.014
	20	5.378 ± 0.015	12.781 ± 0.089	3.421 ± 0.002
	30	5.373 ± 0.025	12.453 ± 0.104	3.407 ± 0.006

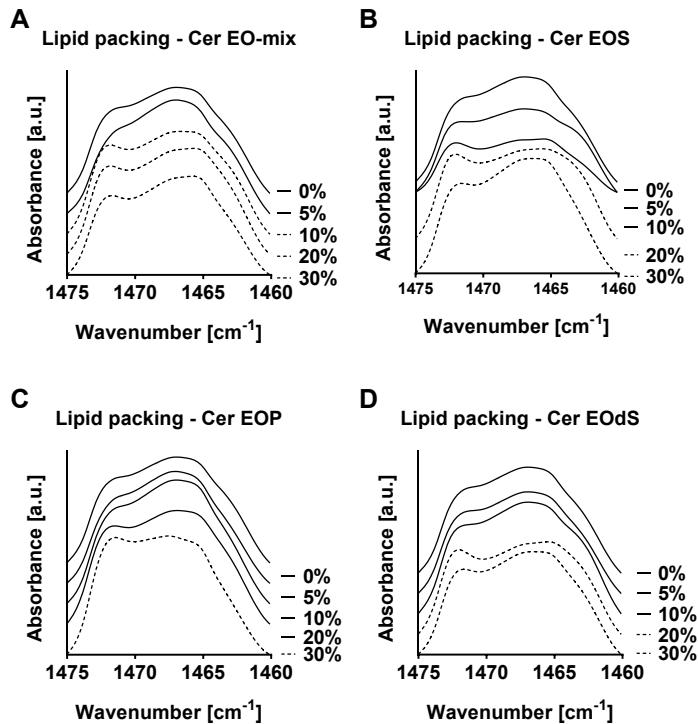
Supplemental Table S1. Repeat distances of the short periodicity phase (SPP), long periodicity phase (LPP) and separated cholesterol (Chol) in membranes containing the acylCer mixture (EO-mix), Cer EOS, EOP and EO_dS. Values are shown as the means ± SEM, n = 4.

acylCer	Molar %	Distance between planes (nm)	
		peak 1	peak 2
Cer EO-mix	--	4.126 ± 0.002	-
	5	4.138 ± 0.005	-
	10	4.141 ± 0.002	3.738 ± 0.005
	20	4.142 ± 0.001	3.750 ± 0.002
	30	4.146 ± 0.001	3.745 ± 0.001
Cer EOS	5	4.140 ± 0.005	-
	10	4.131 ± 0.001	3.729 ± 0.003
	20	4.140 ± 0.001	3.742 ± 0.003
	30	4.142 ± 0.001	3.740 ± 0.002
Cer EOP	5	4.123 ± 0.011	-
	10	4.130 ± 0.009	-
	20	4.147 ± 0.005	3.746 ± 0.006
	30	4.152 ± 0.003	3.751 ± 0.006
Cer EO _d S	5	4.135 ± 0.004	-
	10	4.133 ± 0.004	3.733 ± 0.006
	20	4.139 ± 0.002	3.737 ± 0.002
	30	4.147 ± 0.001	3.740 ± 0.002

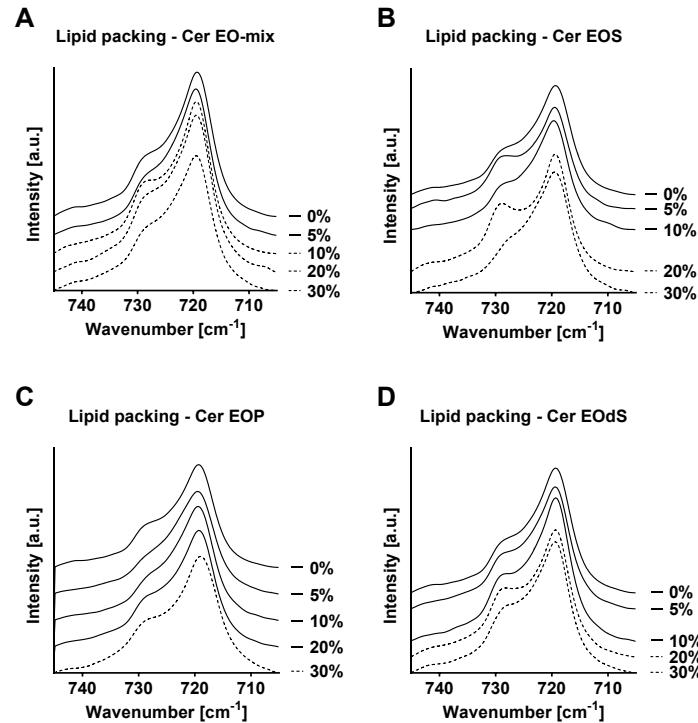
Supplemental Table S2. Position of the two peaks in wide angle X-ray diffraction (WAXD). Values are shown as the means ± SEM, n = 4.



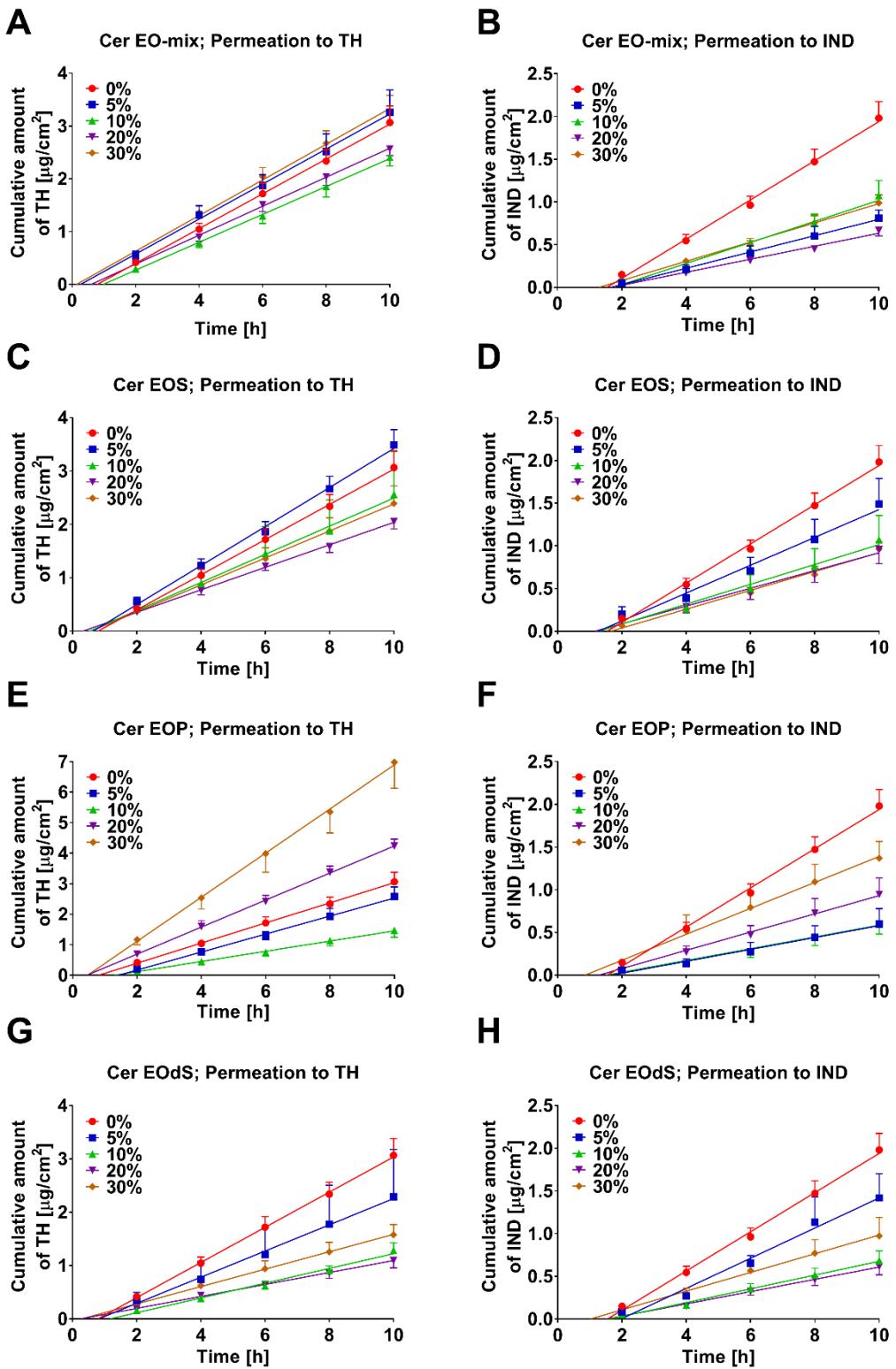
Supplemental Figure S2. Temperature-dependent shift in methylene symmetric stretching vibration showing the main phase transitions of the membranes containing the Cer EO-mix (A), EOS (B), EOP (C) and EO_dS (D). Each curve is shown as the mean \pm SEM, $n = 3$.



Supplemental Figure S3. Methylene scissoring vibration showing the lipid chain packing of membranes containing the Cer EO-mix (A), EOS (B), EOP (C) and EOds (D) (representative spectra).



Supplemental Figure S4. Methylene rocking vibration showing the lipid chain packing of membranes containing the Cer EO-mix (A), EOS (B), EOP (C) and EOds (D) (representative spectra).



Supplemental Figure S5. Cumulative amounts of TH (A, C, E, G) and IND (B, D, F, H) through membranes containing the Cer EO-mix (A+B), EOS (C+D), EOP (E+F) and EOds (G+H). Values are shown as the means \pm SEM, n = 3-10.

Model permeant	acylCer molar %	Flux ($\mu\text{g}/\text{cm}^2/\text{h}$)			
		Cer EO-mix	Cer EOS	Cer EOP	Cer EO _d S
0		0.36 ± 0.04			
TH	5	0.34 ± 0.03	0.37 ± 0.03	0.30 ± 0.04	0.25 ± 0.09
	10	0.25 ± 0.02	0.26 ± 0.07	0.17 ± 0.02	0.14 ± 0.02
	20	0.27 ± 0.02	0.23 ± 0.02	0.44 ± 0.01	0.11 ± 0.01
	30	0.33 ± 0.03	0.25 ± 0.03	0.72 ± 0.09	0.15 ± 0.03
0		0.23 ± 0.02			
IND	5	0.10 ± 0.01	0.16 ± 0.03	0.07 ± 0.02	0.14 ± 0.02
	10	0.12 ± 0.02	0.12 ± 0.03	0.07 ± 0.01	0.08 ± 0.01
	20	0.08 ± 0.01	0.10 ± 0.02	0.11 ± 0.02	0.07 ± 0.01
	30	0.11 ± 0.01	0.11 ± 0.01	0.15 ± 0.02	0.11 ± 0.02

Supplemental Table S3. TH and IND flux values of membranes containing the Cer EO-mix, EOS, EOP and EO_dS. Values are shown as the means \pm SEM, n = 3-10.